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NEWS 8 SEP 25 CAS REGISTRY(SM) no longer includes Concord 3D coordinates
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NEWS 11 OCT 19 LOGOFF HOLD duration extended to 120 minutes
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NEWS 22 DEC 01 CAS REGISTRY updated with new ambiguity codes
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NEWS 24 DEC 14 WPIDS/WPINDEX/WPIX manual codes updated
NEWS 25 DEC 14 GBFULL and FRFULL enhanced with IPC 8 features and functionality
NEWS 26 DEC 18 CA/CAplus pre-1967 chemical substance index entries enhanced with preparation role
NEWS 27 DEC 18 CA/CAplus patent kind codes updated
NEWS 28 DEC 18 MARPAT to CA/CAplus accession number crossover limit increased to 50,000
NEWS 29 DEC 18 MEDLINE updated in preparation for 2007 reload
NEWS 30 DEC 27 CA/CAplus enhanced with more pre-1907 records

NEWS EXPRESS NOVEMBER 10 CURRENT WINDOWS VERSION IS V8.01c, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 25 SEPTEMBER 2006.

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=> E
"N-(4-(3-(4-AMINOPHENYL)-4-ISOAZOLY)PHENYL)-N'-(1-(4-FLUOROPHENYL)ETHYL)THIOUREA"/CN
25
E1           1
N-(4-(3-(4-(MORPHOLIN-4-YL)QUINOLIN-3-YL)ACRYLOYL)PHENYL)OXALAMIC ACID ETHYL
ESTER/CN
E2           1
N-(4-(3-(4-ACETYLPIPERAZIN-1-YL)PROPOXY)NAPHTHALEN-1-YL)-3-FLUORO-5-(PIPERIDIN-1-YL)
BENZAMIDE/CN
E3           0 -->
N-(4-(3-(4-AMINOPHENYL)-4-ISOAZOLY)PHENYL)-N'-(1-(4-FLUOROPHENYL)ETHYL)THIOUREA/CN
E4           1      N-(4-(3-(4-AMINOPHENYL)PROPYL)-1,3-TIAZOL-2-YL)ACETAMIDE/CN
E5           1
N-(4-(3-(4-BENZYLPIPERIDIN-1-YL)PROPYL)PHENYL)-N-(4-HYDROXYBENZYL)BENZENESULFONAMIDE
/CN
E6           1
N-(4-(3-(4-CARBAMIMIDOYLPHENYL)-2-OXOOXAZOLIDIN-5-YLMETHOXY)-3-METHYLNAPHTHALEN-1-YL
)ACETAMIDE/CN

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E7 1
 N-(4-(3-(4-CARBAMIMIDOYLPHENYL)-2-OXOOAZOLIDIN-5-YLMETHOXY)-3-METHYLNAPHTHALEN-1-YL)
)ACETAMIDE ACETATE/CN
 E8 1
 N-(4-(3-(4-CARBAMIMIDOYLPHENYL)-2-OXOOAZOLIDIN-5-YLMETHOXY) PHENYL)ACETAMIDE/CN
 E9 1
 N-(4-(3-(4-CARBAMIMIDOYLPHENYL)-2-OXOOAZOLIDIN-5-YLMETHOXY) PHENYL)ACETAMIDE
 ACETATE/CN
 E10 1
 N-(4-(3-(4-CHLOROBENZENESULFONYL)-4-HYDROXYPHENOXY)-3,5-DIMETHYLPHENYL)OXAMIC
 ACID/CN
 E11 1
 N-(4-(3-(4-CHLOROBENZYLCARBAMOYL)-4-HYDROXYPHENOXY)-3,5-DIMETHYLPHENYL)OXAMIC ACID
 ETHYL ESTER/CN
 E12 1
 N-(4-(3-(4-CHLOROPHENOXY)-4-HYDROXYPHENOXY)-3,5-DIMETHYLPHENYL)OXAMIC ACID/CN
 E13 1
 N-(4-(3-(4-CHLOROPHENYL)-1-OXO-2-PROPEXYL) PHENYL)-2-METHYL-5-NITROBENZENESULFONAMIDE
 /CN
 E14 1
 N-(4-(3-(4-CHLOROPHENYL)BENZO(C)ISOXAZOL-5-YL) PYRIMIDIN-2-YL)ACETAMIDE/CN
 E15 1
 N-(4-(3-(4-CHLOROPHENYL)ISOXAZOL-5-YL) THIAZOL-2-YL)-N-(3-(MORPHOLIN-4-YL) PROPYL) THIO
 PHENE-2-CARBOXAMIDE/CN
 E16 1
 N-(4-(3-(4-CYANO-3-TRIFLUOROMETHYLPHENYL)-5,5-DIMETHYL-4-OXO-2-THIOXOIMIDAZOLIDIN-1-YL)
 PHENYL)ACETAMIDE/CN
 E17 1
 N-(4-(3-(4-CYANO-3-TRIFLUOROMETHYLPHENYL)-5,5-DIMETHYL-4-OXO-2-THIOXOIMIDAZOLIDIN-1-YL)
 PHENYL)METHANESULFONAMIDE/CN
 E18 1
 N-(4-(3-(4-FLUOROBENZENESULFONYL)-4-HYDROXYPHENOXY)-3,5-DIMETHYLPHENYL)-2-MORPHOLIN-
 4-YL-2-OXOACETAMIDE/CN
 E19 1
 N-(4-(3-(4-FLUOROBENZENESULFONYL)-4-HYDROXYPHENOXY)-3,5-DIMETHYLPHENYL)-N'-(2-METHOX
 YETHYL)OXALAMIDE/CN
 E20 1
 N-(4-(3-(4-FLUOROBENZENESULFONYL)-4-HYDROXYPHENOXY)-3,5-DIMETHYLPHENYL)-N'-ISOPROPYL
 OXALAMIDE/CN
 E21 1
 N-(4-(3-(4-FLUOROBENZENESULFONYL)-4-HYDROXYPHENOXY)-3,5-DIMETHYLPHENYL)-N'-PROPYLOXA
 LAMIDE/CN
 E22 1
 N-(4-(3-(4-FLUOROBENZENESULFONYL)-4-HYDROXYPHENOXY)-3,5-DIMETHYLPHENYL)MALONAMIC
 ACID/CN
 E23 1
 N-(4-(3-(4-FLUOROBENZENESULFONYL)-4-HYDROXYPHENOXY)-3,5-DIMETHYLPHENYL)OXALAMIDE/CN
 E24 1
 N-(4-(3-(4-FLUOROBENZENESULFONYL)-4-HYDROXYPHENOXY)-3,5-DIMETHYLPHENYL)OXAMIC
 ACID/CN
 E25 1
 N-(4-(3-(4-FLUOROBENZENESULFONYL)-4-HYDROXYPHENOXY)-3,5-DIMETHYLPHENYL)OXAMIC ACID
 ETHYL ESTER/CN

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=> E

"N-(4-(3-(4-AMINOPHENYL)-4-ISoxAZOLYL) PHENYL)-N'-(1-(4-FLUOROPHENYL) ETHYL) THIOUREA" /
 CN 25

E1 1 N-(4-(3-(4-(MORPHOLIN-4-YL) QUINOLIN-3-YL) ACRYLOYL) PHENYL) OXA
 LAMIC ACID ETHYL ESTER/CN
 E2 1 N-(4-(3-(4-ACETYLPIPERAZIN-1-YL) PROPOXY) NAPHTHALEN-1-YL)-3-F
 LUORO-5-(PIPERIDIN-1-YL) BENZAMIDE/CN
 E3 0 --> N-(4-(3-(4-AMINOPHENYL)-4-ISoxAZOLYL) PHENYL)-N'-(1-(4-FLUORO
 PHENYL) ETHYL) THIOUREA/CN

E4 1 N- (4- (3- (4-AMINOPHENYL) PROPYL) -1, 3-THIAZOL-2-YL) ACETAMIDE/CN
 E5 1 N- (4- (3- (4-BENZYLPIPERIDIN-1-YL) PROPYL) PHENYL) -N- (4-HYDROXYB
ENZYL) BENZENESULFONAMIDE/CN
 E6 1 N- (4- (3- (4-CARBAMIMIDOYLPHENYL) -2-OXOOAZOLIDIN-5-YLMETHOXY)
-3-METHYLNAPHTHALEN-1-YL) ACETAMIDE/CN
 E7 1 N- (4- (3- (4-CARBAMIMIDOYLPHENYL) -2-OXOOAZOLIDIN-5-YLMETHOXY)
-3-METHYLNAPHTHALEN-1-YL) ACETAMIDE ACETATE/CN
 E8 1 N- (4- (3- (4-CARBAMIMIDOYLPHENYL) -2-OXOOAZOLIDIN-5-YLMETHOXY)
PHENYL) ACETAMIDE/CN
 E9 1 N- (4- (3- (4-CARBAMIMIDOYLPHENYL) -2-OXOOAZOLIDIN-5-YLMETHOXY)
PHENYL) ACETAMIDE ACETATE/CN
 E10 1 N- (4- (3- (4-CHLOROBENZENESULFONYL) -4-HYDROXYPHENOXY) -3, 5-DIME
THYLPHENYL) OXAMIC ACID/CN
 E11 1 N- (4- (3- (4-CHLOROBENZYLCARBAMOYL) -4-HYDROXYPHENOXY) -3, 5-DIME
THYLPHENYL) OXAMIC ACID ETHYL ESTER/CN
 E12 1 N- (4- (3- (4-CHLOROPHENOXY) -4-HYDROXYPHENOXY) -3, 5-DIMETHYLPHEN
YL) OXAMIC ACID/CN
 E13 1 N- (4- (3- (4-CHLOROPHENYL) -1-OXO-2-PROPYL) PHENYL) -2-METHYL-5
-NITROBENZENESULFONAMIDE/CN
 E14 1 N- (4- (3- (4-CHLOROPHENYL) BENZO(C) ISOXAZOL-5-YL) PYRIMIDIN-2-YL
) ACETAMIDE/CN
 E15 1 N- (4- (3- (4-CHLOROPHENYL) ISOXAZOL-5-YL) THIAZOL-2-YL) -N- (3- (MO
RPHOLIN-4-YL) PROPYL) THIOPHENE-2-CARBOXAMIDE/CN
 E16 1 N- (4- (3- (4-CYANO-3-TRIFLUOROMETHYLPHENYL) -5, 5-DIMETHYL-4-OXO
-2-THIOXOIMIDAZOLIDIN-1-YL) PHENYL) ACETAMIDE/CN
 E17 1 N- (4- (3- (4-CYANO-3-TRIFLUOROMETHYLPHENYL) -5, 5-DIMETHYL-4-OXO
-2-THIOXOIMIDAZOLIDIN-1-YL) PHENYL) METHANESULFONAMIDE/CN
 E18 1 N- (4- (3- (4-FLUOROBENZENESULFONYL) -4-HYDROXYPHENOXY) -3, 5-DIME
THYLPHENYL) -2-MORPHOLIN-4-YL-2-OXOACETAMIDE/CN
 E19 1 N- (4- (3- (4-FLUOROBENZENESULFONYL) -4-HYDROXYPHENOXY) -3, 5-DIME
THYLPHENYL) -N'-(2-METHOXYETHYL) OXALAMIDE/CN
 E20 1 N- (4- (3- (4-FLUOROBENZENESULFONYL) -4-HYDROXYPHENOXY) -3, 5-DIME
THYLPHENYL) -N'-ISOPROPYLOXALAMIDE/CN
 E21 1 N- (4- (3- (4-FLUOROBENZENESULFONYL) -4-HYDROXYPHENOXY) -3, 5-DIME
THYLPHENYL) -N'-PROPYLOXALAMIDE/CN
 E22 1 N- (4- (3- (4-FLUOROBENZENESULFONYL) -4-HYDROXYPHENOXY) -3, 5-DIME
THYLPHENYL) MALONAMIC ACID/CN
 E23 1 N- (4- (3- (4-FLUOROBENZENESULFONYL) -4-HYDROXYPHENOXY) -3, 5-DIME
THYLPHENYL) OXALAMIDE/CN
 E24 1 N- (4- (3- (4-FLUOROBENZENESULFONYL) -4-HYDROXYPHENOXY) -3, 5-DIME
THYLPHENYL) OXAMIC ACID/CN
 E25 1 N- (4- (3- (4-FLUOROBENZENESULFONYL) -4-HYDROXYPHENOXY) -3, 5-DIME
THYLPHENYL) OXAMIC ACID ETHYL ESTER/CN

=> E

"N1- (4- (3- (4-AMINOPHENYL) -4-ISOXAZOLYL) PHENYL) -N2- (1- (4-FLUOROPHENYL) ETHYL) THIOUREA"
/CN 25
 E1 1 N1- (4- (2, 4-DIMETHYLTHIAZOL-5-YL) PYRIMIDIN-2-YL) -4-METHOXY-N3
, N3-DIMETHYLBENZENE-1, 3-DIAMINE/CN
 E2 1 N1- (4- (2- (4-FLUOROPHENYL) -6-TRIFLUOROMETHYL PYRAZOLO(1, 5-A) PY
RIDIN-3-YL) PYRIMIDIN-2-YL) -N3, N3-DIMETHYLPROPANE-1, 3-DIAMINE
/CN
 E3 0 --> N1- (4- (3- (4-AMINOPHENYL) -4-ISOXAZOLYL) PHENYL) -N2- (1- (4-FLUOR
OPHENYL) ETHYL) THIOUREA/CN
 E4 1 N1- (4- (3-BROMO-4- ((2, 4-DIFLUOROBENZYL) OXY) -6-METHYL-2-OXO-2H
-PYRIDIN-1-YL) BENZYL) -L-SERINAMIDE HYDROCHLORIDE/CN
 E5 1 N1- (4- (3-METHYLCARBAMOYL-4-METHYL-7, 8-METHYLENEDIOXY-3, 4-DIH
YDRO-5H-2, 3-BENZODIAZEPIN-1-YL) PHENYL) -N3-METHYLUREA/CN
 E6 1 N1- (4- (4-AMINO-7- (4-OXOCYCLOHEXYL) -7H-PYRROLO(2, 3-D) PYRIMIDI
N-5-YL) -2-FLUOROPHENYL) -2, 3-DICHLORO-1-BENZENESULFONAMIDE/CN
 E7 1 N1- (4- (4-AMINO-7- (8-METHYL-8-AZA(3.2.1) BICYCLOOCTAN-3-YL) -7H
-PYRROLO(2, 3-D) PYRIMIDIN-5-YL) -2-FLUOROPHENYL) -2, 3-DICHLORO-
1-BENZENESULFONAMIDE/CN
 E8 1 N1- (4- (4-CHLOROPHENOXY) PHENYL) -N, N-DIMETHYLUREA/CN

E9 1 N1-(4-(DIHEXYLAMINO) PHENYL)-N1, N4, N4-TRIHEXYL-1, 4-PHENYLENEDIAMINE/CN
 E10 1 N1-(4-AMINOBUTYL)-N4, N4-BIS (2-HYDROXYETHYL)-2-NITRO-P-PHENYLENEDIAMINE/CN
 E11 1 N1-(4-BROMO-2-((2-FLUOROPHENYL)CARBONYL) PHENYL)-L-ALANINAMIDE/CN
 E12 1 N1-(4-BROMO-2-((2-FLUOROPHENYL)CARBONYL) PHENYL) GLYCINAMIDE/CN
 E13 1 N1-(4-BROMOBENZYL)-N1-(PYRID-2-YL) BUTANE-1, 4-DIAMINE/CN
 E14 1 N1-(4-BROMOPHENYL)-N2-HYDROXY-2-OXO-2-PHENYLACETAMIDINE/CN
 E15 1 N1-(4-BUTOXYBENZYL)-5, 6-DIHYDROTHIOURACIL/CN
 E16 1 N1-(4-CHLOROBENZYL)-4-(3-FLUORO-1-PIPERIDINYL)-4-OXO-1, 3-(S)-BUTANEDIAMINE BIS (TRIFLUOROACETATE)/CN
 E17 1 N1-(4-CHLOROPHENYL)-N3-CYANOQUANIDINE/CN
 E18 1 N1-(4-IMINO-1, 3-DIMETHYL-2, 6-DIOXOHEXAHYDROPYRIMIDIN-5-YL) SULFANILAMIDE/CN
 E19 1 N1-(4-ISOPROPENYLPHENYL)-N3, N3-DIMETHYLSEMICARBAZIDE/CN
 E20 1 N1-(4-ISOPROPOXYBENZOYL)-P-AMINOBENZENESULFONAMIDE/CN
 E21 1 N1-(4-ISOPROPOXYBENZOYL) SULFANILAMIDE/CN
 E22 1 N1-(4-METHYL-2-PYRIDYL) SULFANILAMIDE SODIUM/CN
 E23 1 N1-(4-METHYL-2-PYRIDYL-6-TRIFLUOROMETHYL) SULFANILAMIDE/CN
 E24 1 N1-(4-METHYL-2-PYRIMIDINYL) SULFANILAMIDE/CN
 E25 1 N1-(4-METHYL-2-THIAZOLYL) SULFANILAMIDE/CN

=> E

"N-(4-(3-(4-AMINOPHENYL)-4-ISOXAZOLYL) PHENYL)-N-(1-(4-FLUOROPHENYL) ETHYL) THIOUREA"/CN
N 25

E1 1 N-(4-(3-(4-(MORPHOLIN-4-YL) QUINOLIN-3-YL) ACRYLOYL) PHENYL) OXALAMIC ACID ETHYL ESTER/CN
 E2 1 N-(4-(3-(4-ACETYLPIPERAZIN-1-YL) PROPOXY) NAPHTHALEN-1-YL)-3-FLUORO-5-(PIPERIDIN-1-YL) BENZAMIDE/CN
 E3 0 --> N-(4-(3-(4-AMINOPHENYL)-4-ISOXAZOLYL) PHENYL)-N-(1-(4-FLUOROPHENYL) ETHYL) THIOUREA/CN
 E4 1 N-(4-(3-(4-AMINOPHENYL) PROPYL)-1, 3-THIAZOL-2-YL) ACETAMIDE/CN
 E5 1 N-(4-(3-(4-BENZYLPIPERIDIN-1-YL) PROPYL) PHENYL)-N-(4-HYDROXYBENZYL) BENZENESULFONAMIDE/CN
 E6 1 N-(4-(3-(4-CARBAMIMIDOYLPHENYL)-2-OXOOXAZOLIDIN-5-YLMETHOXY)-3-METHYLNAPHTHALEN-1-YL) ACETAMIDE/CN
 E7 1 N-(4-(3-(4-CARBAMIMIDOYLPHENYL)-2-OXOOXAZOLIDIN-5-YLMETHOXY)-3-METHYLNAPHTHALEN-1-YL) ACETAMIDE ACETATE/CN
 E8 1 N-(4-(3-(4-CARBAMIMIDOYLPHENYL)-2-OXOOXAZOLIDIN-5-YLMETHOXY) PHENYL) ACETAMIDE/CN
 E9 1 N-(4-(3-(4-CARBAMIMIDOYLPHENYL)-2-OXOOXAZOLIDIN-5-YLMETHOXY) PHENYL) ACETAMIDE ACETATE/CN
 E10 1 N-(4-(3-(4-CHLOROBENZENESULFONYL)-4-HYDROXYPHENOXY)-3, 5-DIMETHYLPHENYL) OXAMIC ACID/CN
 E11 1 N-(4-(3-(4-CHLOROBENZYLCARBAMOYL)-4-HYDROXYPHENOXY)-3, 5-DIMETHYLPHENYL) OXAMIC ACID ETHYL ESTER/CN
 E12 1 N-(4-(3-(4-CHLOROPHENOXY)-4-HYDROXYPHENOXY)-3, 5-DIMETHYLPHENYL) OXAMIC ACID/CN
 E13 1 N-(4-(3-(4-CHLOROPHENYL)-1-OXO-2-PROPEXYL) PHENYL)-2-METHYL-5-NITROBENZENESULFONAMIDE/CN
 E14 1 N-(4-(3-(4-CHLOROPHENYL) BENZO(C) ISOXAZOL-5-YL) PYRIMIDIN-2-YL) ACETAMIDE/CN
 E15 1 N-(4-(3-(4-CHLOROPHENYL) ISOXAZOL-5-YL) THIAZOL-2-YL)-N-(3-(MORPHOLIN-4-YL) PROPYL) THIOPHENE-2-CARBOXAMIDE/CN
 E16 1 N-(4-(3-(4-CYANO-3-TRIFLUOROMETHYLPHENYL)-5, 5-DIMETHYL-4-OXO-2-THIOXOIMIDAZOLIDIN-1-YL) PHENYL) ACETAMIDE/CN
 E17 1 N-(4-(3-(4-CYANO-3-TRIFLUOROMETHYLPHENYL)-5, 5-DIMETHYL-4-OXO-2-THIOXOIMIDAZOLIDIN-1-YL) PHENYL) METHANESULFONAMIDE/CN
 E18 1 N-(4-(3-(4-FLUOROBENZENESULFONYL)-4-HYDROXYPHENOXY)-3, 5-DIMETHYLPHENYL)-2-MORPHOLIN-4-YL-2-OXOACETAMIDE/CN
 E19 1 N-(4-(3-(4-FLUOROBENZENESULFONYL)-4-HYDROXYPHENOXY)-3, 5-DIMETHYLPHENYL)-N'-(2-METHOXYETHYL) OXALAMIDE/CN

E20 1 N-(4-(3-(4-FLUOROBENZENESULFONYL)-4-HYDROXYPHENOXY)-3,5-DIME THYLPHENYL)-N'-ISOPROPYLOXALAMIDE/CN
E21 1 N-(4-(3-(4-FLUOROBENZENESULFONYL)-4-HYDROXYPHENOXY)-3,5-DIME THYLPHENYL)-N'-PROPYLOXALAMIDE/CN
E22 1 N-(4-(3-(4-FLUOROBENZENESULFONYL)-4-HYDROXYPHENOXY)-3,5-DIME THYLPHENYL)MALONAMIC ACID/CN
E23 1 N-(4-(3-(4-FLUOROBENZENESULFONYL)-4-HYDROXYPHENOXY)-3,5-DIME THYLPHENYL)OXALAMIDE/CN
E24 1 N-(4-(3-(4-FLUOROBENZENESULFONYL)-4-HYDROXYPHENOXY)-3,5-DIME THYLPHENYL)OXAMIC ACID/CN
E25 1 N-(4-(3-(4-FLUOROBENZENESULFONYL)-4-HYDROXYPHENOXY)-3,5-DIME THYLPHENYL)OXAMIC ACID ETHYL ESTER/CN

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L1 STRUCTURE UPLOADED

=> s 11

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100.0% PROCESSED 0 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
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PROJECTED ITERATIONS: 0 TO 0
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L2 0 SEA SSS SAM L1

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NEWS 18 NOV 10 CA/CAplus F-Term thesaurus enhanced
NEWS 19 NOV 10 STN Express with Discover! free maintenance release Version 8.01c now available
NEWS 20 NOV 20 CAS Registry Number crossover limit increased to 300,000 in additional databases
NEWS 21 NOV 20 CA/CAplus to MARPAT accession number crossover limit increased to 50,000
NEWS 22 DEC 01 CAS REGISTRY updated with new ambiguity codes
NEWS 23 DEC 11 CAS REGISTRY chemical nomenclature enhanced
NEWS 24 DEC 14 WPIDS/WPINDEX/WPIX manual codes updated
NEWS 25 DEC 14 GBFULL and FRFULL enhanced with IPC 8 features and functionality
NEWS 26 DEC 18 CA/CAplus pre-1967 chemical substance index entries enhanced with preparation role
NEWS 27 DEC 18 CA/CAplus patent kind codes updated
NEWS 28 DEC 18 MARPAT to CA/CAplus accession number crossover limit increased to 50,000
NEWS 29 DEC 18 MEDLINE updated in preparation for 2007 reload
NEWS 30 DEC 27 CA/CAplus enhanced with more pre-1907 records

NEWS EXPRESS NOVEMBER 10 CURRENT WINDOWS VERSION IS V8.01c, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 25 SEPTEMBER 2006.

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ENTRY

TOTAL

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STRUCTURE FILE UPDATES 22 DEC 2006 - WHICHET.DAT

DICTIONARY FILE UPDATES: 28 DEC 2006 HIGHEST RN 916479-39-5

STRUCTURE FILE UPDATES: 28 DEC 2006 HIGHEST RN 916479-39-5
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<http://www.cas.org/ONLINE/UG/reaprops.html>

```

=> E
"N-(4-(3-(4-AMINOPHENYL)-4-ISOAZOLY)PHENYL)-N'-(1-(4-FLUOROPHENYL)ETHYL)THIOUREA"/CN
25
E1           1
N-(4-(3-(4-(MORPHOLIN-4-YL)QUINOLIN-3-YL)ACRYLOYL)PHENYL)OXALAMIC ACID ETHYL
ESTER/CN
E2           1
N-(4-(3-(4-ACETYLPIPERAZIN-1-YL)PROPOXY)NAPHTHALEN-1-YL)-3-FLUORO-5-(PIPERIDIN-1-YL)
BENZAMIDE/CN
E3           0 -->
N-(4-(3-(4-AMINOPHENYL)-4-ISOAZOLY)PHENYL)-N'-(1-(4-FLUOROPHENYL)ETHYL)THIOUREA/CN
E4           1      N-(4-(3-(4-AMINOPHENYL)PROPYL)-1,3-TIAZOL-2-YL)ACETAMIDE/CN
E5           1
N-(4-(3-(4-BENZYLPIPERIDIN-1-YL)PROPYL)PHENYL)-N-(4-HYDROXYBENZYL)BENZENESULFONAMIDE
/CN
E6           1
N-(4-(3-(4-CARBAMIMIDOYLPHENYL)-2-OXOOXAZOLIDIN-5-YLMETHOXY)-3-METHYLNAPHTHALEN-1-YL
)ACETAMIDE/CN

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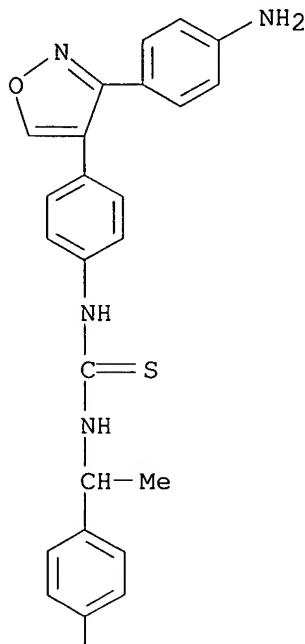
E7 1
N-(4-(3-(4-CARBAMIMIDOYLPHENYL)-2-OXOOAZOLIDIN-5-YLMETHOXY)-3-METHYLNAPHTHALEN-1-YL)
)ACETAMIDE ACETATE/CN
E8 1
N-(4-(3-(4-CARBAMIMIDOYLPHENYL)-2-OXOOAZOLIDIN-5-YLMETHOXY) PHENYL)ACETAMIDE/CN
E9 1
N-(4-(3-(4-CARBAMIMIDOYLPHENYL)-2-OXOOAZOLIDIN-5-YLMETHOXY) PHENYL)ACETAMIDE
ACETATE/CN
E10 1
N-(4-(3-(4-CHLOROBENZENESULFONYL)-4-HYDROXYPHENOXY)-3,5-DIMETHYLPHENYL)OXAMIC
ACID/CN
E11 1
N-(4-(3-(4-CHLOROBENZYLCARBAMOYL)-4-HYDROXYPHENOXY)-3,5-DIMETHYLPHENYL)OXAMIC ACID
ETHYL ESTER/CN
E12 1
N-(4-(3-(4-CHLOROPHENOXY)-4-HYDROXYPHENOXY)-3,5-DIMETHYLPHENYL)OXAMIC ACID/CN
E13 1
N-(4-(3-(4-CHLOROPHENYL)-1-OXO-2-PROPYNYL) PHENYL)-2-METHYL-5-NITROBENZENESULFONAMIDE
/CN
E14 1
N-(4-(3-(4-CHLOROPHENYL) BENZO(C)ISOXAZOL-5-YL) PYRIMIDIN-2-YL)ACETAMIDE/CN
E15 1
N-(4-(3-(4-CHLOROPHENYL) ISOXAZOL-5-YL) THIAZOL-2-YL)-N-(3-(MORPHOLIN-4-YL) PROPYL) THIO
PHENE-2-CARBOXAMIDE/CN
E16 1
N-(4-(3-(4-CYANO-3-TRIFLUOROMETHYLPHENYL)-5,5-DIMETHYL-4-OXO-2-THIOXOIMIDAZOLIDIN-1-YL)
PHENYL)ACETAMIDE/CN
E17 1
N-(4-(3-(4-CYANO-3-TRIFLUOROMETHYLPHENYL)-5,5-DIMETHYL-4-OXO-2-THIOXOIMIDAZOLIDIN-1-YL)
PHENYL)METHANESULFONAMIDE/CN
E18 1
N-(4-(3-(4-FLUOROBENZENESULFONYL)-4-HYDROXYPHENOXY)-3,5-DIMETHYLPHENYL)-2-MORPHOLIN-
4-YL-2-OXOACETAMIDE/CN
E19 1
N-(4-(3-(4-FLUOROBENZENESULFONYL)-4-HYDROXYPHENOXY)-3,5-DIMETHYLPHENYL)-N'-(2-METHOX
YETHYL)OXALAMIDE/CN
E20 1
N-(4-(3-(4-FLUOROBENZENESULFONYL)-4-HYDROXYPHENOXY)-3,5-DIMETHYLPHENYL)-N'-ISOPROPYL
OXALAMIDE/CN
E21 1
N-(4-(3-(4-FLUOROBENZENESULFONYL)-4-HYDROXYPHENOXY)-3,5-DIMETHYLPHENYL)-N'-PROPYLOXA
LAMIDE/CN
E22 1
N-(4-(3-(4-FLUOROBENZENESULFONYL)-4-HYDROXYPHENOXY)-3,5-DIMETHYLPHENYL)MALONAMIC
ACID/CN
E23 1
N-(4-(3-(4-FLUOROBENZENESULFONYL)-4-HYDROXYPHENOXY)-3,5-DIMETHYLPHENYL)OXALAMIDE/CN
E24 1
N-(4-(3-(4-FLUOROBENZENESULFONYL)-4-HYDROXYPHENOXY)-3,5-DIMETHYLPHENYL)OXAMIC
ACID/CN
E25 1
N-(4-(3-(4-FLUOROBENZENESULFONYL)-4-HYDROXYPHENOXY)-3,5-DIMETHYLPHENYL)OXAMIC ACID
ETHYL ESTER/CN

L7 ANSWER 91 OF 177 REGISTRY COPYRIGHT 2007 ACS on STN
 RN 736982-21-1 REGISTRY
 ED Entered STN: 01 Sep 2004
 CN Thiourea, N-[4-[3-(4-aminophenyl)-4-isoxazolyl]phenyl]-N'-(1-(4-fluorophenyl)ethyl)-(9CI) (CA INDEX NAME)
 MF C24 H21 F N4 O S
 SR CA
 LC STN Files: CA, CAPLUS, USPATFULL
 DT.CA CAplus document type: Patent
 RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); USES (Uses)

Ring System Data

Elemental Analysis	Elemental Sequence	Size of the Rings	Ring System Formula	Identifier	Occurrence	RID	Count
EA	ES	SZ	RF	RID			
C3NO	INOC3	15	IC3NO	16.167.5	1		
C6	IC6	16	IC6	46.150.18	3		

PAGE 1-A



PAGE 2-A

|
F

Experimental Property Tags (ETAG)

PROPERTY | NOTE
=====+=====
Mass Spectral(1) CAS

(1) Bloom, Jonathan David; US 2004157900 A1 2004 CAPLUS

Predicted Properties (PPROP)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	1.0	pH 1 25 deg C	(1)
Bioconc. Factor (BCF)	10.28	pH 2 25 deg C	(1)
Bioconc. Factor (BCF)	53.90	pH 3 25 deg C	(1)
Bioconc. Factor (BCF)	90.90	pH 4 25 deg C	(1)
Bioconc. Factor (BCF)	97.57	pH 5 25 deg C	(1)
Bioconc. Factor (BCF)	98.29	pH 6 25 deg C	(1)
Bioconc. Factor (BCF)	98.36	pH 7 25 deg C	(1)
Bioconc. Factor (BCF)	98.36	pH 8 25 deg C	(1)
Bioconc. Factor (BCF)	98.26	pH 9 25 deg C	(1)
Bioconc. Factor (BCF)	97.29	pH 10 25 deg C	(1)
Boiling Point (BP)	583.4+-60.0 deg C	760 Torr	(1)
Density (DEN)	1.309+-0.06 g/cm***3	760 Torr	(1)
Enthalpy of Vap. (HVAP)	87.20+-3.0 kJ/mol	760 Torr	(1)
Flash Point (FP)	306.6+-32.9 deg C		(1)
Freely Rotatable Bonds (FRB)	6		(1)
H acceptors (HAC)	5		(1)
H donors (HD)	4		(1)
Hydrogen Donors/Acceptors Sum (HDAS)	9		(1)
Koc (KOC)	8.42	pH 1 25 deg C	(1)
Koc (KOC)	97.08	pH 2 25 deg C	(1)
Koc (KOC)	508.80	pH 3 25 deg C	(1)
Koc (KOC)	858.08	pH 4 25 deg C	(1)
Koc (KOC)	921.04	pH 5 25 deg C	(1)
Koc (KOC)	927.84	pH 6 25 deg C	(1)
Koc (KOC)	928.52	pH 7 25 deg C	(1)
Koc (KOC)	928.49	pH 8 25 deg C	(1)
Koc (KOC)	927.58	pH 9 25 deg C	(1)
Koc (KOC)	918.43	pH 10 25 deg C	(1)
LOGD (LOGD)	0.88	pH 1 25 deg C	(1)
LOGD (LOGD)	1.94	pH 2 25 deg C	(1)
LOGD (LOGD)	2.66	pH 3 25 deg C	(1)
LOGD (LOGD)	2.89	pH 4 25 deg C	(1)
LOGD (LOGD)	2.92	pH 5 25 deg C	(1)
LOGD (LOGD)	2.92	pH 6 25 deg C	(1)
LOGD (LOGD)	2.92	pH 7 25 deg C	(1)
LOGD (LOGD)	2.92	pH 8 25 deg C	(1)
LOGD (LOGD)	2.92	pH 9 25 deg C	(1)
LOGD (LOGD)	2.92	pH 10 25 deg C	(1)
LOGP (LOGP)	2.925+-0.555	25 deg C	(1)
Mass Intrinsic Solubility (ISLB.MASS)	0.0069 g/L	25 deg C	(1)
Mass Solubility (SLB.MASS)	0.78 g/L	pH 1 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.069 g/L	pH 2 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.013 g/L	pH 3 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.0078 g/L	pH 4 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.0074 g/L	pH 5 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.0069 g/L	pH 6 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.0069 g/L	pH 7 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.0069 g/L	pH 8 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.0069 g/L	pH 9 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.0074 g/L	pH 10 25 deg C	(1)
Mass Solubility (SLB.MASS)	0.0069 g/L	Unbuffered Water	(1)

		pH 7.00	
Molar Intrinsic Solubility (ISLB.MOL)	0.000016 mol/L	25 deg C	(1)
Molar Solubility (SLB.MOL)	0.0018 mol/L	pH 1 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.00016 mol/L	pH 2 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.000030 mol/L	pH 3 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.000018 mol/L	pH 4 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.000017 mol/L	pH 5 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.000016 mol/L	pH 6 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.000016 mol/L	pH 7 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.000016 mol/L	pH 8 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.000016 mol/L	pH 9 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.000017 mol/L	pH 10 25 deg C	(1)
Molar Solubility (SLB.MOL)	0.000016 mol/L	Unbuffered Water	(1)
		pH 7.00	
Molar Volume (MVOL)	330.2+-3.0 cm**3/mol	25 deg C	
		20 deg C	(1)
		760 Torr	
Molecular Weight (MW)	432.51		(1)
PKA (PKA)	12.00+-0.70	Most Acidic	
		25 deg C	
PKA (PKA)	2.91+-0.10	Most Basic	
		25 deg C	
Polar Surface Area (PSA)	108.20 A**2		(1)
Vapor Pressure (VP)	1.34E-13 Torr	25 deg C	(1)

(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software V8.19
 ((C) 1994-2007 ACD/Labs)

See HELP PROPERTIES for information about property data sources in REGISTRY.
 1 REFERENCES IN FILE CA (1907 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 141:190783 CA
 TI Preparation of isoxazole-containing thiourea inhibitors useful for treatment of varicella zoster virus
 IN Bloom, Jonathan David
 PA Wyeth Holdings Corporation, USA
 SO U.S. Pat. Appl. Publ., 9 pp.
 CODEN: USXXCO
 DT Patent
 LA English
 IC ICM C07D261-02
 ICS A61K031-42
 NCL 514378000
 CC 28-6 (Heterocyclic Compounds (More Than One Hetero Atom))
 Section cross-reference(s): 1, 63

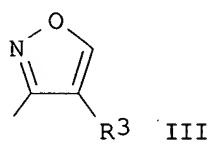
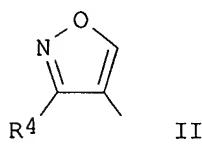
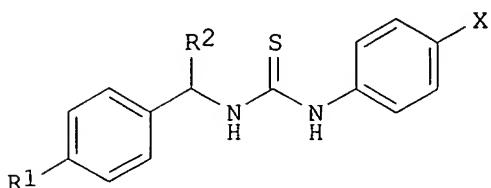
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	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 2004157900	A1	20040812	US 2004-772799	20040205
	WO 2004072052	A2	20040826	WO 2004-US3725	20040209
	WO 2004072052	A3	20041111		
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RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRAI US 2003-446602P 20030211

GI



AB The title compds. [I; R1 = halo, H; R2 = alkyl; X = II, III; R3 = alkyl, cycloalkyl, hydroxymethyl, etc.; R4 = alkyl which may be further substituted with (un)substituted Ph, cycloalkyl, pyridyl, etc.], useful for inhibiting replication of a herpes virus, were prepared E.g., a multi-step synthesis of 1-[4-(4-benzylisoxazol-3-yl)phenyl]-3-[1-(4-fluorophenyl)ethyl]thiourea (IV), was given. Seventeen title compds. I were prepared as described for IV, and tested for activity as herpes virus inhibitors (IC50 values against VZV, MTS, CMV, HSV and RSV were given).

ST isoxazolylphenyl benzyl thiourea prepn antiviral herpes virus; varicella zoster virus isoxazolylphenyl benzyl thiourea prepn

IT Antiviral agents

Human

Human herpesvirus

Human herpesvirus 3

Human herpesvirus 5

(preparation of isoxazole-containing thiourea inhibitors useful for treatment of

varicella zoster virus)

IT Infection

(viral; preparation of isoxazole-containing thiourea inhibitors useful for treatment of varicella zoster virus)

IT 736982-12-0P 736982-13-1P 736982-14-2P 736982-15-3P 736982-16-4P
736982-17-5P 736982-18-6P 736982-19-7P 736982-20-0P 736982-21-1P
736982-22-2P 736982-23-3P 736982-24-4P 736982-25-5P 736982-26-6P
736982-27-7P 736982-28-8P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of isoxazole-containing thiourea inhibitors useful for treatment of

varicella zoster virus)

IT 100-10-7, 4-(Dimethylamino)benzaldehyde 623-04-1, 4-Aminobenzyl alcohol 10147-11-2, 3-Phenyl-1-propyne 14235-81-5, 4-Ethynylaniline 182565-27-1

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of isoxazole-containing thiourea inhibitors useful for treatment of

varicella zoster virus)

IT 2929-84-2P, 4-Dimethylaminobenzaldehyde oxime 144072-29-7P
144072-30-0P 157991-82-7P 170727-03-4P 190446-52-7P 736982-09-5P
736982-10-8P 736982-11-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of isoxazole-containing thiourea inhibitors useful for treatment of

varicella zoster virus)